

# Exact Solutions and hypothesis on Phase Transition in the Polyelectrolite Model of DNA<sup>1</sup>

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The two-dimensional generalization of the Polyelectrolite model of DNA is proposed. It is reduced to the boundary problem for nonlinear quite integrable equation sinh-Gordon. In the linearisable version the exact solution is constructed and its asymptotic is found. The soliton solutions of nonlinear equation are calculated that allowed tells about the possibility of the structural phase transition in the considered system (DNA+polyelectrolite) on the temperature.

At the present time constructing and investigating mathematical models of DNA is an important problem of both theoretical biophysics and mathematical physics. Modern achievements in the field of nonlinear equations theory that occur, as a rule, in these models allow not only to set initial and boundary problems for such equations, but also to solve them in a number of cases.

The given work is devoted to construction of exact solutions for a two-dimensional generalization of so-called polyelectrolyte model of DNA (PM DNA) [1]. In essence here we deal with solution of an inverse problem in the broad sense, i.e. it is to judge structure and properties of a DNA molecule from a field restoring within the framework of this model and also values of some functionals of it.

It is necessary to note that PM represents the most concentrated description of role of Coulomb interactions which are of a great importance in formation of structure of a DNA molecule and in its functioning as well as in intrinsical structural transitions. One more important advantage of the model is possibility to operate with terms of statistical physics, which allows to implement a clear mathematical problem statement.

**The formulation of model and statement of the problem.** In reality a DNA molecule is a strongly charged poly-ion, with two charges of electrons falling at every pair of nucleotides. The idea of PM consists in replacement of such system by an infinite and regular negatively charged cylinder of radius  $r_0$  with a given surface charge density placed into solution of polyelectrolite. It is supposed that a processes of relaxation proceeds quickly enough, so only an equilibrium situation is considered. Besides here we are restricted ourselves by consideration of the case when a solution consists of unitary charged ions and electrons.

Standard physical reasons result to a system of Poisson-Boltzmann equations written down at any point of volume outside the cylinder:

$$\operatorname{div} \mathbf{E} = 4\pi\rho, \quad \mathbf{E} = -\operatorname{grad} U, \quad \rho = e(n_i - n_e), \quad (1)$$

in this case  $n_{i,e}$  being under condition of thermodynamic balance are defined by Boltzmann's distributions:

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$$n_i(U) = n_{0i}e^{-\frac{eU}{T}}, \quad n_e(U) = n_{0e}e^{\frac{eU}{T}}. \quad (2)$$

In formulas (1), (2) the following notations are used:  $\mathbf{E} = \mathbf{E}(x, y, z)$  is a vector of electrical field intensity,  $U = U(x, y, z)$  is a dimensional scalar potential,  $e$  is a charge of electron,  $\rho$  is a charge density,  $n_i$ ,  $n_e$  are concentrations of ions and electrons at the point  $\mathbf{r} = \{x, y, z\}$  correspondingly,  $n_{0i}$ ,  $n_{0e}$  are equilibrium concentrations,  $T$  is absolute temperature, Boltsmann's constant being assumed to be equal to unit.

Supposing that  $n_{0i} = n_{0e} \equiv n_0$  (the condition of total system neutrality) as well as that there is a symmetry in shifting along an axis  $z$  being a symmetry axis of the cylinder, we will pass the plane orthogonal to this axis. Then introducing dimensionless variables  $\mathbf{r}' = \mathbf{r}/(2r_D)$ ,  $u = eU/T$ , where  $r_D$  is Debye radius,  $r_D^2 = T/(8\pi en_0)$ , from (1), (2) we will obtain a basic equation of the model (strokes at independent variables are omitted)

$$\Delta u = 4 \sinh u, \quad (3)$$

where  $\Delta$  is two-dimensional Laplace's operator.

It should be noticed, that the equation (3) also can be obtained from a strict and valid procedure of breakage and disengagement of BBGKI chain in neglecting fluctuations [2,3], with the function  $u$  being an average potential of the system which is a functional of Coulomb's two-partial potential. The equation (3), as applied to PM DNA, corresponds to the case of a salt excess in a polyelectrolyte solution <sup>2</sup>.

$\sinh$ -Gordon equation (3) belongs to the class of two-dimensional completely integrable equations of the elliptical type, for which representation of zero curvature is known [5, 6] and, hence, the Inverse Scattering Transform Method (IST) can be applied. In the papers [7,8] this equation was solved for a half-plane  $y > 0$ , in [9] an IST procedure was employed in solving  $\sinh$ -Gordon-equation fitting Coulomb's system on a plane at negative temperatures, and in a series of papers [10-12] an equation of the same type (with a function  $\sin u$ ) was solved on a whole plane with given conditions on chosen beams (for the purpose of obtaining unambiguous solutions).

Further it will be convenient to work with the equation (3) rewritten in polar coordinates:

$$u_{rr} + \frac{1}{r}u_r + \frac{1}{r^2}u_{\varphi\varphi} = 4 \sinh u, \quad (4)$$

where  $x = r \cos \varphi$ ,  $y = r \sin \varphi$ ,  $r > r_0$  (here  $r_0$  is a dimensionless radius of the cylinder) <sup>3</sup>. Let us assume that  $u = u(r, \varphi)$  is a real-valued function,  $u \rightarrow 0$  with  $r \rightarrow \infty$  quickly enough, with  $u(r, \varphi) = u(r, \varphi + 2\pi)$ .

For (4) are natural two statements of boundary problems:

a) Dirichlet's problem for an exterior of circle:

$$u|_{r=r_0} = \hat{f}_1(\varphi), \quad (5)$$

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<sup>2</sup>If the right part of (3) to substitute for an exponent (having a negative sign both before its argument and before the exponent) will have Liouville's equation having an exact solution [4] that corresponds to a salt lack).

<sup>3</sup>In the one-dimensional case recently this equation has been numerically solved in [13].

b) Neumann's problem for an exterior of circle:

$$u_r|_{r=r_0} = \hat{f}_2(\varphi), \quad (6)$$

in which  $\hat{f}_1(\varphi)$ ,  $\hat{f}_2(\varphi)$  are given periodic functions (linear densities of charges of the cylinder revealing a specific character of DNA molecule).

**Linearized model (a two-dimensional generalization of Debay-Chukkel's model).** At  $r \gg r_0$  the equation (4) can be linearized and then can be written as

$$u_{rr} + \frac{1}{r}u_r + \frac{1}{r^2}u_{\varphi\varphi} = 4u.$$

Taking  $u = u(r, \varphi) = R(r)\Phi(\varphi)$ , we shall have

$$r^2 R_{rr} + r R_r - (4r^2 + \lambda)R = 0, \quad \Phi_{\varphi\varphi} + \lambda\Phi = 0, \quad (7)$$

where a parameter  $\lambda \in \mathbb{C}$ . Considering a finiteness of solution from (7) we find:

$$u(r, \varphi) = \sum_m b_m K_m(2r) e^{im\varphi}, \quad \lambda = m^2. \quad (8)$$

where  $b_m$  are constants,  $K_m(\cdot)$  are modified Bessel functions (McDonald's functions), and the summation is over  $m$  within limits from  $-\infty$  to  $+\infty$ . In the case of the problem (5) coefficients  $b_m$  are defined from the condition

$$b_m = \frac{1}{2\pi K_m(2r_0)} \int_0^{2\pi} d\varphi \hat{f}_1(\varphi) e^{-im\varphi}.$$

Thus, we obtain

$$u(r, \varphi) = \frac{1}{2\pi} \int_0^{2\pi} d\varphi' \sum_m e^{im(\varphi-\varphi')} \frac{K_m(2r)}{K_m(2r_0)} \hat{f}_1(\varphi'). \quad (9)$$

Similarly in the case of a problem (6) we find

$$u(r, \varphi) = \sum_m c_m K_m(2r) e^{im\varphi}, \quad \lambda = m^2,$$

and the coefficients  $c_m$  are defined by relations

$$c_m = -\frac{1}{2\pi} \frac{\int_0^{2\pi} d\varphi \hat{f}_2(\varphi) e^{-im\varphi}}{K_{m-1}(2r_0) + K_{m+1}(2r_0)}.$$

Hence it follows that

$$u(r, \varphi) = -\frac{1}{2\pi} \int_0^{2\pi} d\varphi' \sum_m e^{im(\varphi-\varphi')} \frac{K_m(2r)}{K_{m-1}(2r_0) + K_{m+1}(2r_0)} \hat{f}_2(\varphi'). \quad (10)$$

It is easy to show that both (9) and (10) meets the requirement of reality. Representations (9) and (10) are solutions of Debay-Chukkel's two-dimensional theory corresponding to anisotropic medium (polyelectrolyte), which can arise owing to, for example, possible (probable) fluctuations in the system.

Fourier-factors  $\hat{f}_{1m}, \hat{f}_{2m}$  of expansion of functions  $\hat{f}_1(\varphi), \hat{f}_2(\varphi)$ , are obviously connected by the relations:  $\hat{f}_{1m}/K_m(2r_0) = \hat{f}_{2m}/(2K'_m(2r_0))$ , which allows to establish a nonlocal relation <sup>4</sup>):

$$u_r(r_0, \varphi) = \int_0^{2\pi} d\varphi' H(r_0, \varphi - \varphi') u(r_0, \varphi'), \quad (11)$$

in which the function  $H(r_0, \varphi)$  is determined by the equality:

$$H(r_0, \varphi) = \frac{1}{\pi} \sum_m \frac{K'_m(2r)}{K_m(2r_0)} e^{im\varphi}.$$

Using (9) and the Fourier-factors connection (11) established above we obtain

$$u(r, \varphi) = \frac{1}{4\pi} \int_0^{2\pi} d\varphi' \sum_m e^{im(\varphi - \varphi')} K_m(2r) \left[ \frac{\hat{f}_1(\varphi')}{K_m(2r_0)} + \frac{\hat{f}_2(\varphi')}{2K'_m(2r_0)} \right].$$

Returning to (8), where

$$b_m = \frac{1}{2\pi} \int_0^{2\pi} d\varphi e^{-im\varphi} \left[ \frac{u(r_0, \varphi)}{K_m(2r_0)} + \frac{u_r(r_0, \varphi)}{2K'_m(2r_0)} \right],$$

and considering that  $b_{-m} = \bar{b}_m$ , we have

$$u(r, \varphi) = u_0(r) + 4 \sum_{m=1}^{\infty} (\text{Re } b_m) K_m(2r) \cos m\varphi, \quad (12)$$

with  $u_0(r) = b_0 K_0(2r)$ ,  $b_0 = \bar{b}_0$ . The formula (12) is convenient for obtaining asymptotic representations. Then

$$u_0(r) \sim \frac{b_0}{\sqrt{\pi r}} e^{-2r}, \quad r \rightarrow \infty.$$

Thus, we can deduce a relation describing an effect of Debye screening. Putting

$$u^+(r, \varphi) = \sum_{m=1}^{\infty} \tilde{b}_m K_m(2r) e^{im\varphi}, \quad \tilde{b}_m = 4 \text{Re } b_m,$$

and assuming the possibility of analytic continuation of  $\tilde{b}_m$  on an index  $m$ , we convert a last sum in integral in the ordinary way:

$$u^+(r, \varphi) = \int_C ds \frac{\tilde{b}_s e^{i(\pi + \varphi)s}}{2i \sin \pi s} K_s(2r), \quad (13)$$

where a contour of integration starts from an infinite (along  $\text{Re } s$ ) point located in the first quarter of the complex variable  $s$  plane, then goes parallel to the real axis crossing it at the point  $0 < \text{Re } s < 1$ , and then ends at infinity parallel to the real axis and remaining in the fourth quarter.

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<sup>4</sup>The idea of the approach belongs to V.D.Lipovsky.

To calculation an asymptotic form of the expression (13) it should be applied the saddle-point method. For that at first we should notice that the function  $K_s$  satisfies the equation

$$K_{s,rr} + \frac{1}{r}K_{s,r} - (4 + \frac{m^2}{r^2})K_s = 0. \quad (14)$$

Taking  $\xi = 2r$ ,  $K_s = f_s/\sqrt{\xi}$ , we reduce (14) to the form

$$f_s'' - (\frac{m^2 - \frac{1}{4}}{\xi^2} + 1)f_s = 0.$$

From here it follows that

$$K_s(\xi) \sim \sqrt{\frac{2}{\pi\xi}} \left( \frac{s^2 - \frac{1}{4}}{\xi^2} + 1 \right)^{-\frac{1}{4}} \exp \left\{ -\sqrt{1 + \frac{\xi^2}{s^2 - \frac{1}{4}}} + \frac{1}{2} \ln \frac{\sqrt{1 + \frac{\xi^2}{s^2 - \frac{1}{4}}} - 1}{\sqrt{1 + \frac{\xi^2}{s^2 - \frac{1}{4}}} + 1} \right\},$$

or, after simple calculations (assuming  $s/\xi = o(1)$ ,  $\xi \rightarrow \infty$ ),

$$K_s(2r) \sim \frac{1}{\sqrt{\pi r}} e^{-2r} e^{-\frac{s^2}{4r}}, \quad r \rightarrow \infty.$$

Then it is possible to rewrite (13) as:

$$u^+(r, \varphi) \sim \frac{1}{\sqrt{\pi r}} e^{-2r} \int_C ds \frac{\tilde{b}_s}{2i \sin \pi s} e^{is(\pi + \varphi) - \frac{s^2}{4r}}, \quad r \rightarrow \infty. \quad (15)$$

Let us assume that  $s = s_0\xi$ ,  $s_0 = 2i(\pi + \varphi)r$ . Then a whole picture will be turned through a corner -  $\pi/2$ : the poles will turned out in the negative part of the imaginary axis, and the integration contour  $C$  will turn into a contour  $C'$  beginning at the point  $a - i\infty$ , going parallel to the imaginary axis and then crossing it and finally ending at the point  $-a - i\infty$  remaining parallel of the axis, where  $a$  is a positive constant. Assuming that "factors"  $\tilde{b}_s$  permit an analytic continuation to required areas of the lower semiplane, instead of (15) we obtain

$$u^+(r, \varphi) \sim \frac{1}{\sqrt{\pi r}} e^{-2r} s_0 \int_{C'} d\xi \frac{\tilde{b}(s_0\xi)}{2i \sin[2i\pi(\pi + \varphi)r\xi]} e^{-r(\pi + \varphi)^2(2\xi - \xi^2)}, \quad r \rightarrow \infty.$$

On introducing a function  $G(\xi) = \xi^2 - 2\xi$  we find the saddle point:  $\xi_0 = 1$ ; then in its vicinity  $G(\xi) = -1 + (\xi - \xi_0)^2 + O((\xi - \xi_0)^3)$ . Deforming the contour in such a way that it goes through the saddle point in the direction of the steepest descent, we have

$$u^+(r, \varphi) = \left\{ \frac{\tilde{b}(2i(\pi + \varphi)r)}{\sinh[2r\pi(\pi + \varphi)]} (1 + O(\frac{1}{r})) \right\} e^{-[2 + (\pi + \varphi)^2]r}, \quad r \rightarrow \infty.$$

This expression, which is the leading member of the asymptotic form, gives an amendment to the effect of Debye screening on plane.

**Exact solutions and "soliton" configurations of the equation (4).** Let us proceed to constructing exact solutions of the equation (4). It should be notice that the

solution of the boundary problems (4), (5) or (4), (6) encounters serious mathematical difficulties involving application of IST (a scattering problem for the operator of an associated linear problem on half-axis). Therefore here we should be restricted by a more simple problem: in neglecting the radius  $r_0$  we will construct exact solutions of (4) on a whole plane by means of Darboux Transformation (DT) method.

Employing a direct calculation it is possible to check up that the equation (4) is a condition of compatibility of the overdetermined linear matrix system

$$\Psi_r = U\Psi, \quad \Psi_\varphi = rV\Psi, \quad (16)$$

where  $\Psi = \Psi(r, \varphi, \lambda)$ ,  $U = U(r, \varphi, \lambda)$ ,  $V = V(r, \varphi, \lambda) \in Mat(2, \mathbb{C})$ ,  $\lambda \in \mathbb{C}$  is a parameter, and the matrixes  $U$ ,  $V$  are given as <sup>5</sup>:

$$U(r, \varphi, \lambda) = \frac{i\lambda}{2}e^{i\varphi}\sigma_3 + \frac{\cosh u}{2i\lambda}e^{-i\varphi}\sigma_3 - \frac{u_r - \frac{i}{r}u_\varphi}{4}\sigma_2 - \frac{\sinh u}{2\lambda}e^{-i\varphi}\sigma_1,$$

$$V(r, \varphi, \lambda) = -\frac{\lambda}{2}e^{i\varphi}\sigma_3 - \frac{\cosh u}{2\lambda}e^{-i\varphi}\sigma_3 - i\frac{u_r - \frac{i}{r}u_\varphi}{4}\sigma_2 - \frac{\sinh u}{2i\lambda}e^{-i\varphi}\sigma_1.$$

Here  $\sigma_i$ ,  $i = 1, 2, 3$ , are Pauli's standard matrixes.

Further instead of variable  $r$ ,  $\varphi$  it is convenient to introduce the "conic" variables  $\zeta = (\varphi + i \ln r)/2$ ,  $\bar{\zeta} = (\varphi - i \ln r)/2$ , and also using invariance of a condition of compatibility of the system (16) relative to a cyclic rearrangement of Pauli's matrixes, it is worth changing to the another its gauge. Then instead of (16) we have the following  $2 \times 2$  matrix system

$$\Psi_\zeta = A\Psi, \quad \Psi_{\bar{\zeta}} = B\Psi, \quad (17)$$

where

$$A = A(\zeta, \bar{\zeta}, \lambda) = \frac{1}{\lambda}e^{-2i\zeta} \begin{pmatrix} 0 & e^u \\ e^{-u} & 0 \end{pmatrix}, \quad B = B(\zeta, \bar{\zeta}, \lambda) = \begin{pmatrix} \frac{u_{\bar{\zeta}}}{2} & \lambda e^{2i\bar{\zeta}} \\ \lambda e^{2i\zeta} & -\frac{u_{\bar{\zeta}}}{2} \end{pmatrix}.$$

The compatibility condition (17) becomes  $A_{\bar{\zeta}} - B_{\zeta} + [A, B] = 0$ , and an appropriate nonlinear equation, takes the form

$$u_{\zeta\bar{\zeta}} = 4 \sinh u e^{-2i(\zeta - \bar{\zeta})},$$

which, as it is easy to show, is equivalent to (4).

Let  $\Psi = (\Psi^{(1)}, \Psi^{(2)})$ ,  $\Psi^{(1)} = (\theta, \chi)^T$ . Then the equations system (17) can be written as a system of four equations

$$\theta_\zeta = \frac{e^u}{\lambda}e^{-2i\zeta}\chi, \quad \chi_\zeta = \frac{e^{-u}}{\lambda}e^{-2i\zeta}\theta, \quad (18)$$

$$\theta_{\bar{\zeta}} = \frac{u_{\bar{\zeta}}}{2}\theta + \lambda e^{2i\bar{\zeta}}\chi, \quad \chi_{\bar{\zeta}} = \lambda e^{2i\bar{\zeta}}\theta - \frac{u_{\bar{\zeta}}}{2}\chi.$$

Let  $\theta_1$ ,  $\chi_1$  be a fixed solution of (18) corresponding to the choice  $\lambda = \lambda_1$ . Let us assume

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<sup>5</sup>For the first time these expressions were obtained by S.S. Nikulichev

$$\tilde{\theta} = \lambda\chi - \lambda_1 \frac{\chi_1}{\theta_1} \theta, \quad \tilde{\chi} = \lambda\theta - \lambda_1 \frac{\theta_1}{\chi_1} \chi,$$

and check up covariance of the system (18) relative to DT of a such form. After simple calculations it can be obtained

$$\tilde{u} = u + 2 \ln \frac{\chi_1}{\theta_1}. \quad (19)$$

In the theory of DT the relation is called a "dressing" one.

To construction an explicit solution it is necessary to assign some initial one; here as the solution we choose  $u = 0$ . Turning back to polar coordinates, then from system (18) we obtain

$$\theta_{1r} = -\frac{1}{2i} [\cos \varphi (\frac{1}{\lambda_1} - \lambda_1) - i \sin \varphi (\frac{1}{\lambda_1} + \lambda_1)] \chi_1, \quad (20)$$

$$\theta_{1\varphi} = \frac{1}{2} r [\cos \varphi (\frac{1}{\lambda_1} + \lambda_1) - i \sin \varphi (\frac{1}{\lambda_1} - \lambda_1)] \chi_1.$$

The given system has an integral:  $\theta_1^2 - \chi_1^2 = A_1^2$ , where  $A_1$  is an arbitrary, generally speaking, complex constant, which allows to integrate (20). We have

$$\chi_1 = \frac{1}{2} A_1 (e^{\Gamma_1 - \ln A_1} - e^{-\Gamma_1 + \ln A_1}), \quad \theta_1 = \frac{1}{2} A_1 (e^{\Gamma_1 - \ln A_1} + e^{-\Gamma_1 + \ln A_1}).$$

Here  $\Gamma_1 = -1/(2i) [\cos \varphi (1/\lambda_1 - \lambda_1) - i \sin \varphi (1/\lambda_1 + \lambda_1)] r + \ln B_1$ ,  $B_1$  is a real constant (for simplicity  $A_1$  is considered to be real as well).

Considering (19), it is can be seen that the potential becomes real at  $\lambda_1 = e^{i\alpha_1}$ ,  $\alpha_1 \in \mathbb{R}$ ,  $\alpha_1 \in [0, 2\pi]$ . Then the simplest solution of the equations (4) takes the form ( $u[1] \equiv \tilde{u}$ )

$$u[1] = 2 \ln \{ \tanh[r \sin(\varphi + \alpha_1) + \delta_1] \}, \quad (21)$$

where  $\delta_1 = \ln |B_1/A_1|$ . The solution (21) is an analogue of the solution type of 1-kink for nonlinear equations of the hyperbolic type [5] and describes a distribution of the potential on plane. Also it is of interest to note that in solving the equation (3) on half-plane by means of IST, 1-kink solutions turn out to be forbidden because of the potential must be real [8].

Let us consider an double dressing procedure for the initial solution. Repeating procedure of obtainment (19) we have

$$u[2] = u + 2 \ln \frac{\chi_1 \chi_2[1]}{\theta_1 \theta_2[1]}. \quad (22)$$

Here

$$\begin{aligned} \theta_2[1] &= e^{-2i\bar{\zeta}} (\theta_{2\bar{\zeta}} - \frac{\theta_{1\bar{\zeta}}}{\theta_1} \theta_2) = \lambda_2 \chi_2 - \lambda_1 \frac{\chi_1}{\theta_1} \theta_2, \\ \chi_2[1] &= e^{-2i\bar{\zeta}} (\chi_{2\bar{\zeta}} - \frac{\chi_{1\bar{\zeta}}}{\chi_1} \chi_2) = \lambda_2 \theta_2 - \lambda_1 \frac{\theta_1}{\chi_1} \chi_2, \end{aligned}$$

and  $\chi_2 = \chi_2(r, \varphi)$ ,  $\theta_2 = \theta_2(r, \varphi)$  are solutions of the system (20) for  $\lambda = \lambda_2$ . Then the relation (22) can be rewritten in the form

$$u[2] = u + 2 \ln \frac{\lambda_2 \chi_1 \theta_2 - \lambda_1 \theta_1 \chi_2}{\lambda_2 \chi_2 \theta_1 - \lambda_1 \chi_1 \theta_2}. \quad (23)$$

On examining reality of the expression (23) it can be resulted in two possible cases.

1. Let  $\lambda_k = e^{i\alpha_k}$ ,  $\alpha_k \in [0, 2\pi]$ ,  $k = 1, 2$ , i.e. both complex parameters must belong to an unit circle <sup>6</sup>. Let us assume  $\Gamma_k = r \sin(\varphi + \alpha_k) + \ln B_k$ ,  $B_k \in \mathbb{R}$ ,  $k = 1, 2$ , and as solutions of the system (34) take

$$\chi_k = C_k e^{\Gamma_k + \ln \delta_k} + i D_k e^{-\Gamma_k - \ln \delta_k}, \quad \theta_k = C_k e^{\Gamma_k + \ln \delta_k} - i D_k e^{-\Gamma_k - \ln \delta_k}.$$

In this case the reality is guaranteed provided  $\chi_k = \bar{\theta}_k$ ,  $C_k, D_k \in \mathbb{R}$ ,  $-4i C_k D_k = A_k^2$ , and then we obtain:

$$u_{ks}[2] = 2 \ln \frac{1 + h_{ks}}{1 - h_{ks}}, \quad h_{ks} = h(r, \varphi) = -\cot Q \frac{\sinh(\Gamma_2 - \Gamma_1 + \nu_1)}{\cosh(\Gamma_1 + \Gamma_2 + \nu_2)}. \quad (24)$$

Here  $\nu_1 = \ln |\delta_2/\delta_1| - (1/2) \ln |R_1/R_2|$ ,  $\nu_2 = \ln |\delta_1\delta_2| + (1/2) \ln |R_1 R_2|$ ,  $\delta_1, \delta_2 \in \mathbb{R}$ ,  $R_k = D_k/C_k$ ,  $q = (\alpha_1 - \alpha_2)/2$ .

The solution (24) is an analogue of 2-kinks solution for equations of the hyperbolic type. It differs a little from a solution of the equation (3) obtained in [8] for half-plane by means of IST (ibidem the appropriate asymptotic forms at  $r \rightarrow \infty$  have been found).

2. Let  $\lambda_1 = \gamma_1 e^{i\alpha_1}$ ,  $\lambda_2 = 1/\bar{\lambda}_1$ ,  $\alpha_1, \gamma_1 \in \mathbb{R}$ ,  $\alpha_1 \in [0, 2\pi]$ ,  $\gamma_1 > 0$ . Then  $\Gamma(\lambda_1) = \bar{\Gamma}(\lambda_2)$ ,  $\Gamma(\lambda_1) \equiv \Gamma_1 = -1/(2i)[\cos \varphi(1/\lambda_1 - \lambda_1) - i \sin \varphi(1/\lambda_1 + \lambda_1)]r = \Gamma_{1R} + i\Gamma_{1I}$ ,  $\Gamma_{1R} = (1/2) \sin(\varphi + \alpha_1)(1/\gamma_1 + \gamma_1)r$ ,  $\Gamma_{1I} = (1/2) \cos(\varphi + \alpha_1)(\gamma_1 - 1/\gamma_1)r$ . Setting  $\theta_1 = \bar{\chi}_2$ ,  $\theta_2 = \bar{\chi}_1$ ,  $k = 1, 2$ , where  $\chi_k = F_k e^{\Gamma_k} - G_k e^{-\Gamma_k}$ ,  $\theta_k = F_k e^{\Gamma_k} + G_k e^{-\Gamma_k}$ , we have the other real solution:

$$u_b[2] = 2 \ln \frac{1 - h_b}{1 + h_b}, \quad h_b = h(r, \varphi) = \cot(\ln \gamma_1) \frac{\sin[2 \cos(\varphi + \alpha_1)(\sinh \gamma_1)r]}{\cosh[2 \sin(\varphi + \alpha_1)(\cosh \gamma_1)r + \mu_1]}. \quad (25)$$

Here  $F_k, G_k \in \mathbb{R}$ ,  $4F_k G_k = A_k^2$ ,  $A_k^2 \in \mathbb{R}$ ,  $\mu_1 = (1/2) \ln[(F_1^2 + F_2^2)/(G_1^2 + G_2^2)]$ .

The formula (25) is an analogue of the solution type of breather (a double soliton) for a hyperbolic equation. In [8] the solution has been obtained by help of IST and its asymptotic forms have been calculated.

Procedure of obtaining subsequent "dressing" relations is same as in deducing (23) (see, for example, [14]), and also results in  $N$  - "soliton" solutions.

**On Phase Transition in PM DNA.** In the context of the problem under examination a rather wide solutions spectrum calculated above can be interpreted as one answering to various parameters or, perhaps, to various states of DNA. It allows, in particular, to put forward a hypothesis about a probable (within the framework of a used model) structural phase of transition of the 2-nd sort on temperature (for example, type of spiral  $\rightarrow$  ball or B-form  $\rightarrow$  Z-form, where B and Z are right and left spiral DNA accordingly). Such a transition is possible due to our system is two-dimensional one (it should be reminded

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<sup>6</sup>Employing IST for half-plane it has been shown that a parameter  $\lambda$  has sense of a spectral parameter for an associated linear problem (16) [7,8] whereas values  $\lambda_k$  form its discrete spectrum.



that, according to Landau [15], such changes are forbidden in one-dimensional systems). As its mechanism the following one can be considered.

Let two complex parameters (an eigen values) forming an inversion relative to an unit circle in the plane of a complex parameter  $\lambda$  (state of the "breather" type) are available. It is assumed that in the system some change of temperature occurs, so that given parameters become dependent on it. It means that they start moving along the beam drawing between them (on the complex plane). In bringing together in the vicinity of the unit circle "a scattering" of the parameters occurs one on the other, and as a result they either with some probability  $p = p(\alpha, T)$  drift apart along the circle, or with the probability  $1-p$  "pass" through each other in such a way as to keep forming inversion relative to the circle obeying requirement of reality of the potential. The temperature, at which the phenomenon take places, is critical for the process; and the process corresponds to a structural phase of transition of the 2-nd sort <sup>7</sup>. In order to prove this, following the idea of Landau, we are to calculate free energies of 2-kinks and breather configurations in the vicinity of the critical temperature and obtain a (nonzero) jump of the second derivative with respect to a free energy on temperature.

However, there is one essential difficulty. The point is that according to so-called Derrick's theorem, in two-dimension systems a functional of energy turns out to be infinite (see [16], where questions on stability of integrable equations solutions have been detailed considered as well). Therefore to estimate the free energy functional, strictly speaking, it is to employ some mathematically correct procedure. Nevertheless, we suggest quite a simple (and correct, in our opinion) technique allowing to avoid this difficulty.

Let us identify a free energy with a generating functional of the model (4):

$$\begin{aligned}\mathcal{F}(u) &= \int \int_{\{\mathbb{R}^2 \setminus C_{r=r_0}\}} dx dy \left\{ 4(\cosh u - 1) + \frac{1}{2}(u_x^2 + u_y^2) \right\} = \\ &= \int_{r=r_0}^{\infty} \int_0^{2\pi} dr d\varphi r \left\{ 4(\cosh u - 1) + \frac{1}{2}(u_r^2 + \frac{1}{r^2}u_\varphi^2) \right\},\end{aligned}$$

where a symbol  $\{\mathbb{R}^2 \setminus C_{r=r_0}\}$  means that one integrates over the space  $\mathbb{R}^2$  with a remote circle of radius  $r_0$ . Using the representations (24) or (25) for a function  $u = u(r, \varphi)$ , we reduce  $\mathcal{F}(u)$  to the form convenient for subsequent estimations:

$$\mathcal{F}(u) = 8 \int_{r=r_0}^{\infty} \int_0^{2\pi} dr d\varphi r \frac{4h^2 + h_r^2 + \frac{h_\varphi^2}{r^2}}{(1+h)^2(1-h)^2}. \quad (26)$$

Here an auxiliary function  $h = h(r, \varphi)$  satisfies a nonlinear (and also, as well as (4)) a completely integrable equation

$$h_{rr} + \frac{1}{r^2}h_{\varphi\varphi} + \frac{2(h_r^2 + \frac{h_\varphi^2}{r^2})}{1-h^2} + \frac{h_r}{r} = \frac{4h(1+h^2)}{1-h^2},$$

whose representation of a zero curvature can be obtained from the conditions of system compatibility (16).

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<sup>7</sup>In other words, here the phase of transition is connected to an asymptotical degeneration of eigen values, and the potential plays a part of the ordering parameter.

According to the critical phenomena theory [17,18], close to the critical point it is to assume  $\gamma_1 = \gamma_1(t) = e^{v_1}$ , where  $v_1 = v_1(t) \sim t^{d_1}$ ,  $t = (T_* - T)/T_*$ ,  $d_1$  is the critical factor,  $d_1 > 0$ ,  $T_*$  is the critical temperature. Then a simple estimation for  $h = h_b$  near  $T = T_*$  gives

$$h_b \sim \frac{1}{v_1} \frac{\sin[2 \cos(\varphi + \alpha_1) \hat{C}_1 r]}{\cosh[2 \cos(\varphi + \alpha_1) \hat{C}_2 r + \mu_1]} \equiv \frac{1}{v_1} F_b(r, \varphi), \quad v_1 \rightarrow 0.$$

Here  $\hat{C}_1, \hat{C}_2$  is a real constant.

Operating analogously for a condition characterizing by two "kinks", on setting  $v_2 \equiv (\alpha_1 - \alpha_2)/2 \sim t^{d_2}$ , where  $d_2$  a critical factor also,  $d_2 > 0$ , we find ( $\Phi = \varphi + (\alpha_1 + \alpha_2)/2$ )

$$h_{ks} \sim -\frac{1}{v_2} \frac{\sinh \nu_1}{[\cosh \nu_2 + \sinh(2r \sin \Phi) \sinh \nu_2]} \equiv \frac{1}{v_2} F_{ks}(r, \varphi), \quad v_2 \rightarrow 0.$$

Thus, from (26) one can obtain

$$\mathcal{F}_b(t, r_0) \sim v_1^2 Q_b(r_0), \quad \mathcal{F}_{ks}(t, r_0) \sim v_2^2 Q_{ks}(r_0),$$

where  $Q_b(r_0), Q_{ks}(r_0)$  are expressions that can be resulted in by what ever way of regularization of corresponding integrals. From here it follows that

$$\frac{(\mathcal{F}_b)_{TT}}{(\mathcal{F}_{ks})_{TT}} = \frac{Q_b}{Q_{ks}} \frac{d_1}{d_2} \frac{2d_1 - 1}{2d_2 - 1} t^{2(d_2 - d_1)}.$$

Assuming  $d_2 - d_1 = O(t)$  at  $T \nearrow T_*$  and eliminating an uncertainty available here, we have

$$(\mathcal{F}_b)_{TT|T=T_*} \neq (\mathcal{F}_{ks})_{TT|T=T_*},$$

and, thus, we show that at the critical point the existence of a change of phase of the 2-nd sort is possible (this qualitative conclusion, certainly, does not depend on a way of regularization). It should be also noticed that exact values of the critical factors can be determined on obtaining identities of traces arising in analyzing an appropriate spectral problem (in [8] the values for half-plane have turned out to be equal to  $1/2$ ).

**Conclusion.** In the present paper an exact solution for Debay-Chukkel's two-dimensional model has been constructed and its asymptotic form has been found as well. In the nonlinear case by means of Darboux Transformation method exact solutions have been calculated and a hypothesis about an possibility of a change of phase has been put forward and checked. Note that we did not solve a boundary problem for the equations (4), as such, because IST, generally speaking, is not adapted for this procedure<sup>8</sup>. Therefore a conclusion about existence of a change of phase has, as a whole, a preliminary character. Besides a number of other important questions arising in the framework of PM such as question about thermodynamics of investigated system, about changes of phase corresponding to more complex soliton solutions, about methods of functionals regularization and others have not been considered either but will be discussed in future.

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<sup>8</sup>Recently some progress in this direction has been achieved in [19] for a hyperbolic version of sin-Gordon equation.

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